
2. TECHNICAL SUMMARY AND BACKGROUND

2.1 Overview of QUAL2E

QUAL-I was initially developed by the Texas Water Development Board in the 1960s. Several improved versions of the model were developed by EPA as part of this effort, and after extensive review and testing the QUAL-II series became widely used. Present support for the model is provided by the Environmental Protection Agency's Center for Exposure Assessment Modeling (CEAM).

QUAL2E simulates up to 15 water quality constituents in branching stream systems. The model uses a finite-difference solution of the advective-dispersive mass transport and reaction equations. A stream reach is divided into a number of computational elements, and for each computational element, a hydrologic balance in terms of stream flow (e.g., m^3/s), a heat balance in terms of temperature (e.g., $^{\circ}C$), and a material balance in terms of concentration (e.g., mg/l) are written. Both advective and dispersive transport processes are considered in the material balance. Mass is gained or lost from the computational element by transport processes, wastewater discharges, and withdrawals. Mass can also be gained or lost by internal processes such as release of mass from benthic sources or biological transformations.

The program simulates changes in flow conditions along the stream by computing a series of steady-state water surface profiles. The calculated stream-flow rate, velocity, cross-sectional area, and water depth serve as a basis for determining the heat and mass fluxes into and out of each computational element due to flow. Mass balance determines the concentrations of conservative minerals, coliform bacteria, and nonconservative constituents at each computational element. In addition to material fluxes, major processes included in mass balance are transformation of nutrients, algal production, benthic and carbonaceous demand, atmospheric reaeration, and the effect of these processes on the dissolved oxygen balance. QUAL2E uses chlorophyll *a* as the indicator of planktonic algae biomass. The nitrogen cycle is divided into four compartments: organic nitrogen, ammonia nitrogen, nitrite nitrogen, and nitrate nitrogen. In a similar manner, the phosphorus

cycle is modeled by using two compartments. The primary internal sink of dissolved oxygen in the model is biochemical oxygen demand (BOD). The major sources of dissolved oxygen are algal photosynthesis and atmospheric reaeration.

The model is applicable to dendritic streams that are well mixed. It assumes that the major transport mechanisms, advection and dispersion, are significant only along the main direction of flow (the longitudinal axis of the stream or canal). It allows for multiple waste discharges, withdrawals, tributary flows, and incremental inflow and outflow. It also has the capability to compute required dilution flows for flow augmentation to meet any pre-specified dissolved oxygen level.

Hydraulically, QUAL2E is limited to the simulation of time periods during which both the stream flow in river basins and input waste loads are essentially constant. QUAL2E can operate as either a steady-state or a quasi-dynamic model, making it a very helpful water quality planning tool. When operated as a steady-state model, it can be used to study the impact of waste loads (magnitude, quality, and location) on instream water quality. By operating the model dynamically, the user can study the effects of diurnal variations in meteorological data on water quality (primarily dissolved oxygen and temperature) and also can study diurnal dissolved oxygen variations due to algal growth and respiration. However, the effects of dynamic forcing functions, such as headwater flows or point loads, cannot be modeled in QUAL2E.

2.2 Prototype Presentation

Prototype representation in QUAL2E consists of dividing a stream into a network consisting of "Headwater," "Reaches," and "Junctions." The fundamental reason for subdividing sections of a stream into "reaches" is that QUAL2E assumes that some 26 physical, chemical, and biological parameters (model input parameters or coefficients) are constant along a "reach." For example, different values for Manning's roughness coefficient, sediment oxygen demand, and algal settling rate can be specified by the user for different reaches, but each of these values remains

constant over a particular reach. However, the state variables change within a reach; e.g., DO is calculated at each computational element and thus can vary within a reach. The question that must be addressed in order to define a "reach" is what constitutes "significant" change in these model inputs—"significant" in the sense of their impact on simulation results, not necessarily in the sense of change in the inputs themselves.

Mass transport in the QUAL2E computer program is handled in a relatively simple manner. There seems to be some confusion about QUAL2E's transport capabilities because it is sometimes called a "quasi-dynamic" model. However, in all of the computer programs in the QUAL series, there is an explicit assumption of steady flow; the only time-varying forcing functions are the climatologic variables that primarily affect temperature and algal growth. A more appropriate term for this capability is "diel," indicating variation over a 24-hour period. The forcing function used for estimating transport is the stream flow rate, which, as mentioned above, is assumed to be constant. Stream velocity, cross-sectional area, and depth are computed from stream flow.

One of the most important considerations in determining the assimilative capacity of a stream is its ability to maintain an adequate dissolved oxygen concentration. The QUAL2E program performs dissolved oxygen balance by including major source and sink terms in the mass balance equation. As shown in Figure 2.1, the nitrogen cycle is composed of four compartments: organic nitrogen, ammonia nitrogen, nitrite nitrogen, and nitrate nitrogen. The phosphorus cycle is similar to, but simpler than, the nitrogen cycle, having only two compartments. Ultimate carbonaceous biochemical oxygen demand (CBOD) is modeled as a first-order degradation process in QUAL2E. If the modeler uses BOD5 as an input, QUAL2E converts 5-day BOD to ultimate BOD for internal calculations. Oxidation processes involved in CBOD decay and in the nutrient cycles represent the primary internal sinks of dissolved oxygen in the QUAL2E program. The major source of dissolved oxygen, in addition to that supplied from algal photosynthesis, is atmospheric reaeration.

2.3 Uncertainty Analysis

Uncertainty analysis for model simulations is assuming a growing importance in the field of water quality management. QUAL2E allows the modeler to perform uncertainty analysis on steady-state water quality simulations. Three uncertainty analysis tech-

niques are employed in QUAL2E-UNCAS: sensitivity analysis, first-order error analysis, and Monte Carlo simulation. With this capability, the user can assess the effect of model sensitivities and of uncertain input data on model forecasts. Quantifications of the uncertainty in model forecasts will allow assessment of the risk (probability) of a water quality variable being above or below an acceptable level. The user can select the important input variables to be perturbed and locations on the stream where the uncertainty analysis is to be applied.

2.4 Data Requirements

QUAL2E requires some degree of modeling sophistication and expertise on the part of a user. The user must supply more than 100 individual inputs, some of which require considerable judgment to estimate. The input data in QUAL2E can be grouped into three categories: a stream/river system, global variables, and forcing functions. Additionally, there are three data groups for simulation control and uncertainty analysis.

The first step in preparing the QUAL2E inputs is to describe a complete stream/river system by applying the rules that are defined by the model. The stream system should be divided into reaches, which are stretches of stream that have uniform hydraulic characteristics. Each reach is then subdivided into computational elements of equal length. Thus, all reaches must consist of an integer number of computational elements. Functionally each computational element belongs to one of seven types (described later). River reaches are the basis of most input data.

The global variables include simulation variables, such as units and simulation type, water quality constituents, and some physical characteristics of the basin. Up to 15 water quality constituents can be modeled by QUAL2E.

Forcing functions are user-specified inputs that drive the system being modeled. These inputs are specified in terms of flow, water quality characteristics,

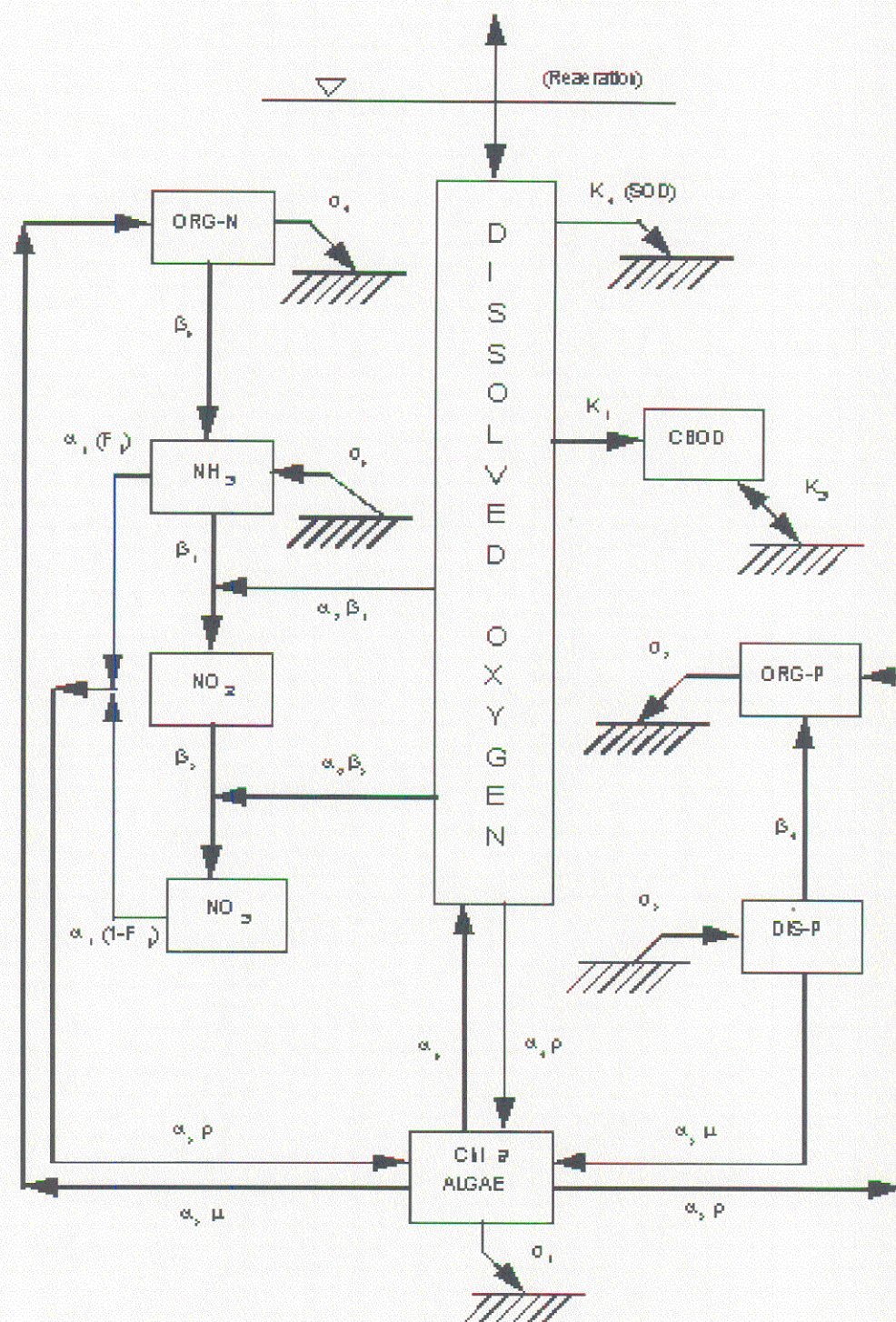


Figure 2.1 QUAL2E Constituent Interactions

and local climatology. QUAL2E accommodates four types of hydraulic and mass-load-forcing functions in addition to local climatological factors: headwater inputs, point sources or withdrawals, incremental inflow/outflow along a reach, and the downstream boundary concentration (optional).

Local climatological data are required for the simulation of algae and temperature. The temperature simulation uses a heat balance across the air-water interface and thus requires values of wet and dry bulb air temperatures, atmospheric pressure, wind velocity, and cloud cover. The algal simulation requires values of net solar radiation. For dynamic simulations, these climatological data must be input at regular time intervals over the course of the simulation and are applied uniformly over the entire river basin. For modeling steady-state temperature and algae, average daily local climatological data are required and may vary spatially over the basin by reach.

The uncertainty analysis procedures incorporated into the computer program guide the user in the calibration process, in addition to providing information about the uncertainty associated with the calibrated model.

To create QUAL2E input files, the user has to follow data type sequences within one particular input file. There are five different input files for which certain combinations must be created before running the model.

2.5 Output File

QUAL2E produces three types of tables—hydraulics, reaction coefficient, and water quality—in the output file. The hydraulics summary table contains flows, velocities, travel time, depths, and cross-sectional areas along each reach. The reaction coefficient table lists the reaction coefficients for simulated constituents. The water quality table reports constituent concentrations along a reach. A summary of temperature calculations may also be included.

2.6 Model Limitations

QUAL2E has been designed to be a relatively general program; however, certain dimensional limitations were imposed during program development (Brown and Barnwell, 1987). These limitations are:

- Reaches: a maximum of 50
- Computational elements: no more than 20 per reach or a total of 500
- Headwater elements: a maximum of 10
- Junction elements: a maximum of 9
- Point source and withdrawal elements: a maximum of 50